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A Study of Quantum Bistability

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Abstract

We report the preliminary results of a numerical simulation of bistable switching in a one dimensional resonant system within the mean-field approximation. The problem is intriguing because of the peculiarity of the existence of a non-unique transport properties of the system, although the scattering states of the potential is expected to be unique.

1. Introduction

The appearance of bistable transport properties in quantum transport is intriguing, however a common occurrence. The transport properties may be derived from an analysis of the scattering states of the corresponding potential[1], which are expected to be unique. On the other hand, simple approximations such as the treatment of the interparticle potential within self-consistent mean-field theory easily yield bistability, and the phenomenon is easily observed experimentally. The problem has a qualitative similarity to the observation of metastable states in first order phase transitions: A complete theoretical description of the states is not straightforward, but they may be obtained trivially within a mean-field theoretical treatment, and again observed quite readily experimentally. It is of fundamental interest to understand whether the quantum mechanical bistability may be understood within the framework of a many-particle scattering theory, or whether it is necessary to include additional mechanisms (such as dissipation) into the formalism in order to obtain the multi-valued transport properties. Indeed it is not clear whether the observed states themselves actually correspond to the time independent scattering solutions of the quantum mechanical problem, or whether they are "metastable" in some sense as in the case of the phase transition analogy.

Bistability is also of interest due to its potential for applications. Besides the obvious possible application for information storage, the switching process between the bistable states is one of few ways to obtain a fast response to a slow external perturbation.

In the present work, we report the results of a numerical simulation of the bistable switching process between the two bistable states of the current-voltage characteristics of a one-dimensional double-barrier resonant geometry using the time dependent Schrödinger equation[2]. An ensemble of particles, interacting through a model repulsive potential are coupled to the system through absorbing and injecting boundary conditions corresponding to reservoirs. The potential is assumed to exist only in the resonance region and is determined through a self-consistent mean-field potential approximation. The implementation of the injecting and absorbing boundary conditions on the contacts is not straightforward, and a method that we have developed earlier[3] was used in the simulation. The Fermi energies at the two "contacts" to the system are changed adiabatically to obtain the current through the system as a function of the potential difference.

For a system being brought to the switching region, it is observed that the current tends to "hang" in the original state for some period of time, the duration of which depends dramatically on the potential difference. However, once the current starts changing towards the other bistable value, the switching waveform is remarkably uniform and swift, and does not depend on the applied potential difference. The switching speed does however depend on the physical parameters (such as the strength of the inter-particle interaction) that define the resonance region, and slows down appreciably as the bistability disappears. This slowing down is reminiscent of the critical slowing down associated with critical phenomena, and a naive analysis of the slowing down indicates an inverse power law scaling of the time constant as a function of the aforementioned parameters.

2. The Model

The system that has been studied is shown in Figure-1. A double barrier structure

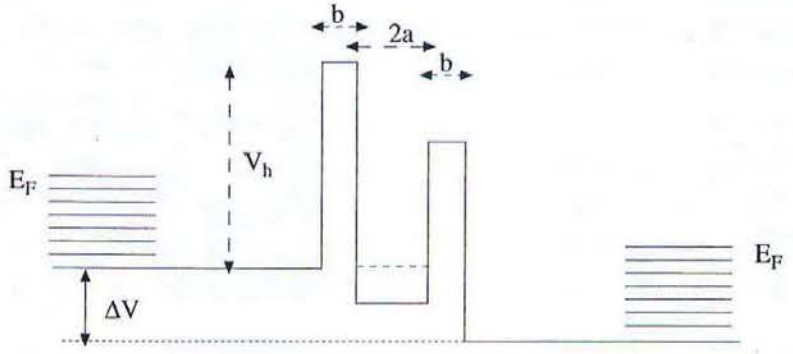

Figure 1. The double barrier model whose transport properties are studied. Various geometry parameters are discussed in the text.

results in a resonance for certain incident wavelengths of particles. An ensemble of 40 to 80 particles with equally spaced energies and with magnitudes scaled to unity are incident from both sides of the geometry. This corresponds to a Fermi distribution of energies at zero temperature. Each particle interacts with others via an additional constant potential,

only in the region between the barriers, determined self consistently and with a magnitude proportional to the total magnitude of the other particles present in this region:

$$V_j(x) = \begin{cases} \beta \sum_{k \neq j} \int' \psi^*{}_k(x')\psi_k(x')dx' & \text{for } x \text{ between barriers} \\ 0 & \text{otherwise .} \end{cases} \tag{1}$$

Here, V_j is the potential acting on the jth particle, ψ_k is the wave function corresponding to the kth particle, and β is a parameter that adjusts the strength of the inter-particle coupling. The prime on the integral indicates that the x' integral is to be evaluated only in the space between the barriers. The mean field approach allows the decoupling of the system so that it may be studied in terms of single particle states.

Extensive details of the simulation will not be given here, the interested reader is referred to references [2] and [3] for the details of how the integration of the Schrödinger equation is carried out, as well as the numerical implementation of the injecting and absorbing boundary conditions. It will be emphasized however that the problem of the boundary conditions is not trivial, and an accurate implementation permits the time dependent analysis. The simulation is carried on a one-dimensional mesh of 127 points. For any chosen physical mesh length of Δx, one may normalize the energy scale by the quantity $\epsilon_0 = \hbar^2/2m^*(\Delta x)^2$, with m^* the effective mass of the particles. (For "reasonable" values of Δx = 10nm and m^* =$0.067m_e$ corresponding to GaAs, $\epsilon_0 \approx$0.57eV.) The time may also be scaled by the quantity $\tau = \hbar/\epsilon_0$ ($\approx$1.2fs for GaAs). In this work, the barriers, and the distance between the barriers were taken to be one and five mesh units respectively. The barrier potential was taken to be 0.9 and the Fermi energy at the contacts were taken to be 0.14 in these units.

The current through the structure was calculated as the superposition of the currents that are being carried by the individual particles. The potential energy difference between the minimum energies at the two contacts (the "bias") V was varied from 0 (where no bistability is expected) to 1 very slowly, and then back to 0 to observe the possible switching phenomena and the eventual steady state current flowing through the system.

For each strength of the inter-particle coupling strength β that was studied in the simulation, the time independent solution of Schrödinger equation at zero potential difference and no inter-particle interaction was taken as the initial condition of the system. After a sufficient amount simulation at "zero bias" in order to achieve a steady current flow, the potential was changed adiabatically, at a rate much slower than the speed of the bistable switching mechanism. We have also studied the effects of changing the potential difference abruptly to the instability region to isolate the effects of slower processes.

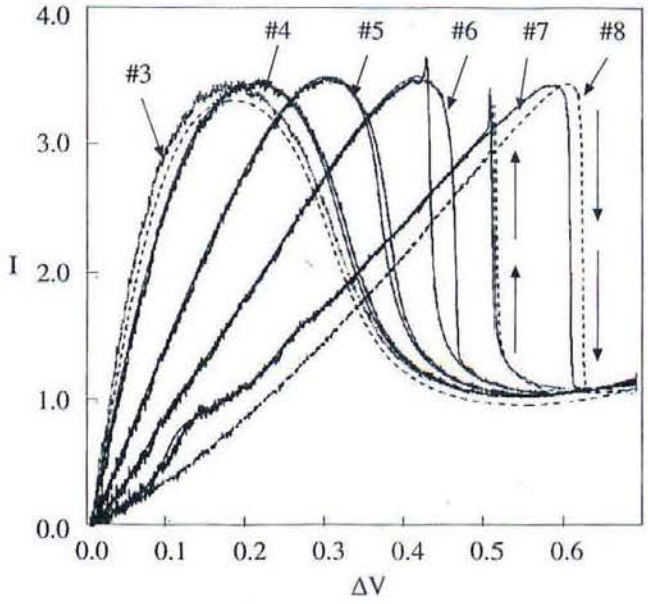

Figure 2. The current as a function of potential difference across the structure for various values of the inter-particle coupling parameter β. The curves identified as #3 through #8 correspond to values of β =0, 0.0002, 0.0009, 0.002, 0.004, and 0.004 respectively. Curve #8 corresponds to a simulation with a total of 80 particles, others to 40 particles. The dashed curve next to the $\beta = 0$ result corresponds to the solution of the time independent equation with a 800 particle ensemble.

3. Results and Conclusions

The simulation was tested against the time independent calculations in the special case $\beta = 0$. (Curve number 3 and the associated dashed curve in Figure-2.) No bistability was observed in this case, as expected. But as the inter-particle interaction strength β is increased, a hysteresis loop is observed in the current - voltage relationship as one increases the potential difference across the bistability region, and decreases back to zero bias. Figure-2 displays the onset of bistability, with the very thin hysteresis evident for β equal to 0.0002 and 0.0009 probably corresponding to the slowing down of the response of the system (reminiscent of the critical slowing down analogy) and the resulting "non-adiabaticity" of the potential variation procedure due to this.

Figure-3 displays a more detailed look at the bistable switching process. For this figure, the potential difference across the geometry was kept constant once it reaches the value indicated. The figure displays the amount of total charge between the barriers as a function of time. There is an initial, potential independent, relaxation to a "waiting" state. This feature is related to the small amount of non-adiabaticity due the variation of the potential, and corresponds to the settling down of the system to its (possibly metastable) steady state. Unlike the metastable states corresponding to the mean field theory descriptions of phase transitions (in which all possible fluctuations out of these

states are suppressed), the quantum mechanical system may tunnel out of this state to the stable one. This tunneling, or "waiting" time depends on the potential difference at which the system is held, as is apparent in Figure-3. There is a range of potential differences for which there is true bistability, where there are two possible values for the transport

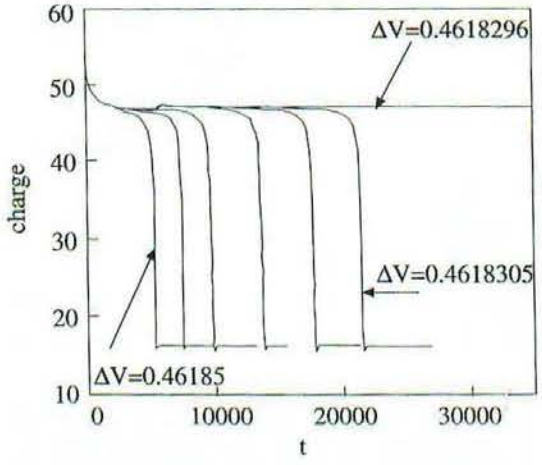

Figure 3. The "waiting" and switching behavior of the charge between the barriers for the inter-particle coupling $\beta = 0.002$ while the potential difference across the structure is kept constant. The value of this potential difference for the curves not identified on the figure is 0.4618400, 0.4618370, 0.4618337, and 0.4618315.

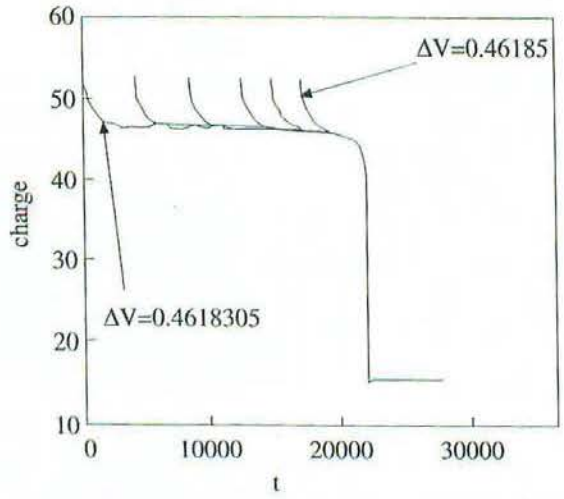

Figure 4. The curves in Figure 3, redrawn to display the common switching behavior.

properties of the system. Outside this range, once the system dynamics of switching has reached a certain point, there is (again, a potential independent) change to the stable state. In Figure-4, the same curves have been re-drawn with appropriate shifts to display

the overlap in this relatively faster switching regime. This switching speed in turn is a function of the parameters that define the extent of bistability, such as the inter-particle coupling β and the geometry of the structure. Figure-5 shows that this rate is remarkably linear as a function of the inter-particle coupling, and seems to go to zero at the onset of bistability, reminiscent of critical slowing down.

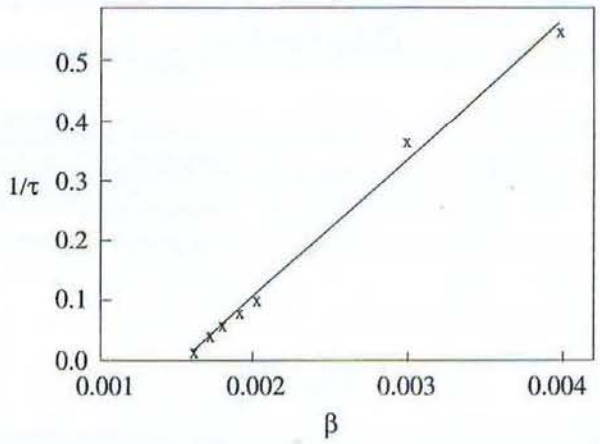

Figure 5. The inverse of the switching time as a function of the inter-particle coupling.

We have reported results from a numerical simulation of bistability in a double barrier resonant structure with a mean-field treatment of inter-particle coupling. The problem has at least some qualitative similarities to the problem of metastable states in first order phase transitions. It would be interesting to study similar systems with higher levels of accuracy in order to see the actual extent of this similarity. The challenge remains for obtaining a fundamental explanation of bistability in quantum transport, its nature and the basic mechanisms that are responsible for it.

References

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